

2-(Difluoromethoxy)-1,1,1,3,3,3-hexafluoropropane  
26103-08-2 | DTXSID60448843

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 41.7

Global applicability domain: Inside

Local applicability domain index: 3.08e-01

Confidence level: 6.50e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1,1,1,3,3,3-Hexafluoro-2-propanol</div> <div>Measured: 2.51</div> <div>Predicted: 2.40</div>	<div>Image not found</div> <div>Benzotrifluoride</div> <div>Measured: 44.7</div> <div>Predicted: 13.7</div>	<div>Image not found</div> <div>Dichlorodifluoromethane</div> <div>Measured: 6.17</div> <div>Predicted: 9.03</div>
<div>Image not found</div> <div>3-Chlorobenzotrifluoride</div> <div>Measured: 224</div> <div>Predicted: 317</div>	<div>Image not found</div> <div>2,4-Dichlorobenzotrifluoride</div> <div>Measured: 2340</div> <div>Predicted: 108</div>	